

# High-Order Shock-Capturing Methods for Study of Shock-Induced Turbulent Mixing with Adaptive Mesh Refinement Simulations

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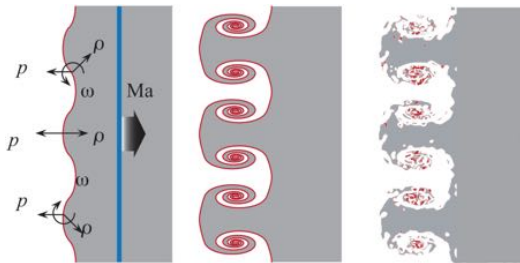
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# Motivation

- **Richtmyer-Meshkov (RM) instability**, or **RMI**, occurs when a shock wave passes through a perturbed interface separating two fluids with different densities
- In natural phenomena/engineering applications:
  - Supernova explosion (SNe)
  - Inertial confinement fusion (ICF)
  - Supersonic combustion in scramjet



RMI evolution (Image Credit: B. M. Wilson, R. Mejia-Alvarez and K. P. Prestridge)



Supernova remnant (Image Credit: NASA/ESA/HEIC and The Hubble Heritage Team (STScI/AURA))

# Motivation

- A lack of understanding of turbulent mixing induced from RMI, due to:
  - Only simultaneous measurements of density and velocity fields in 2D<sup>1 2</sup>
  - Direct numerical simulations still too expensive
  - Methods to save computational cost:
    - High-order shock-capturing schemes
    - Adaptive gridding for localized and mobile features (shocks, mixing regions, etc.)
- High-order numerical schemes with adaptive mesh refinement (AMR) still not very popular for RMI simulations:
  - Tritschler et al.<sup>3</sup> used high-order schemes with uniform grid to study RMI with re-shock
  - Grinstein and Gowardhan<sup>4</sup> used AMR but only second order scheme for RMI simulations
  - McFarland et al.<sup>5</sup> also used second order scheme with AMR for inclined interface RMI

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<sup>1</sup> Mohammad Mohaghar et al. "Evaluation of turbulent mixing transition in a shock-driven variable-density flow". In: *Journal of Fluid Mechanics* 831 (2017), pp. 779–825.

<sup>2</sup> Daniel T Reese et al. "Simultaneous direct measurements of concentration and velocity in the Richtmyer–Meshkov instability". In: *Journal of Fluid Mechanics* 849 (2018), pp. 541–575.

<sup>3</sup> VK Tritschler et al. "On the Richtmyer–Meshkov instability evolving from a deterministic multimode planar interface". In: *Journal of Fluid Mechanics* 755 (2014), pp. 429–462.

<sup>4</sup> FF Grinstein, AA Gowardhan, and AJ Wachtor. "Simulations of Richtmyer–Meshkov instabilities in planar shock-tube experiments". In: *Physics of Fluids* 23.3 (2011), p. 034106.

<sup>5</sup> Jacob A McFarland, Jeffrey A Greenough, and Devesh Ranjan. "Computational parametric study of a Richtmyer–Meshkov instability for an inclined interface". In: *Physical Review E* 84.2 (2011), p. 026303.

# Motivation

- Goals of research:
  - Numerical framework for simulations of RMI and similar types of flows. The framework combines:
    - Improved high-order shock-capturing methods to preserve fine-scales better
    - AMR technique that only applies fine grid cells around localized features
  - Study the turbulent mixing induced by RMI through simulations:
    - Variable-density mixing effects
    - Effects of Reynolds number
    - Analyze the performance of reduced-order modeling through second-moment closures

# Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows
2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability
3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock
4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability

# Weighted compact nonlinear schemes (WCNS's): governing equation

- Consider a scalar conservation law for 1D problem:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

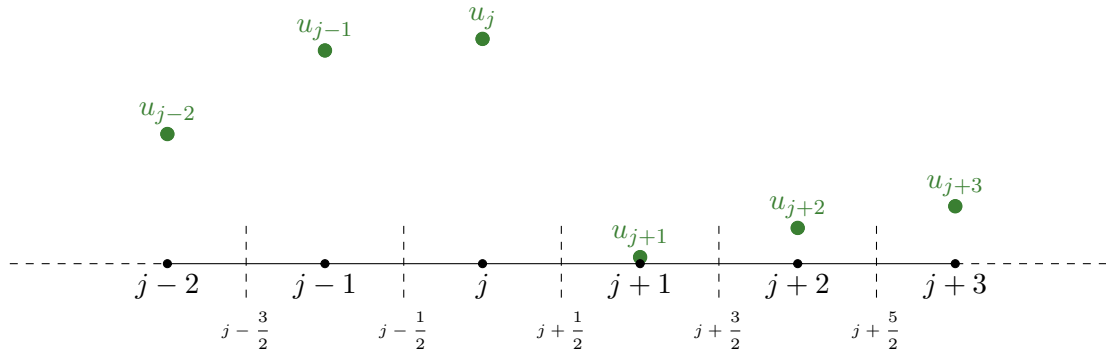
- Semi-discretize this equation on a grid with  $N$  points:

$$\frac{\partial u_j}{\partial t} + \frac{\partial f(u)}{\partial x} \Big|_j = 0$$

- Need a discrete approximation of the flux derivative:

$$\frac{\partial f(u)}{\partial x} \Big|_j$$

# Illustration of methodology of WCNS's <sup>6 7</sup>

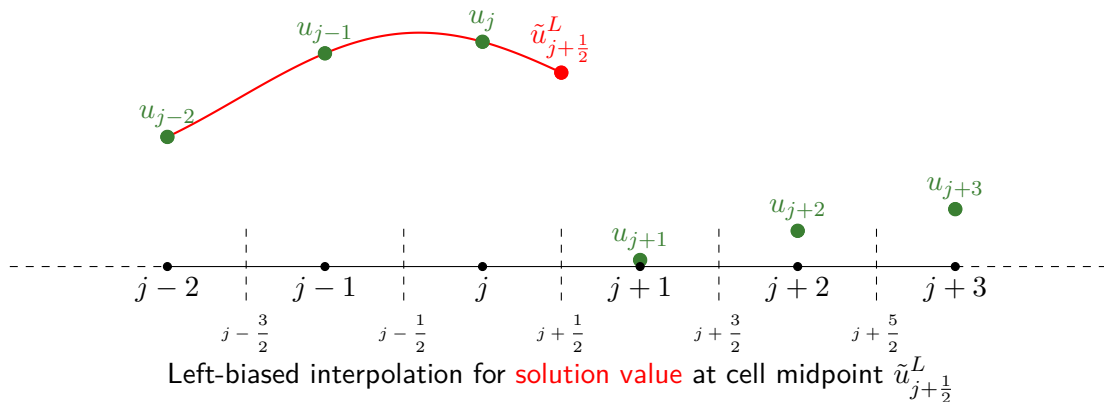


Given the **solution values** at cell nodes

<sup>6</sup>Xiaogang Deng and Hanxin Zhang. "Developing high-order weighted compact nonlinear schemes". In: *Journal of Computational Physics* 165.1 (2000), pp. 22–44.

<sup>7</sup>Shuhai Zhang, Shufen Jiang, and Chi-Wang Shu. "Development of nonlinear weighted compact schemes with increasingly higher order accuracy". In: *Journal of Computational Physics* 227.15 (2008), pp. 7294–7321.

# Illustration of methodology of WCNS's <sup>6 7</sup>

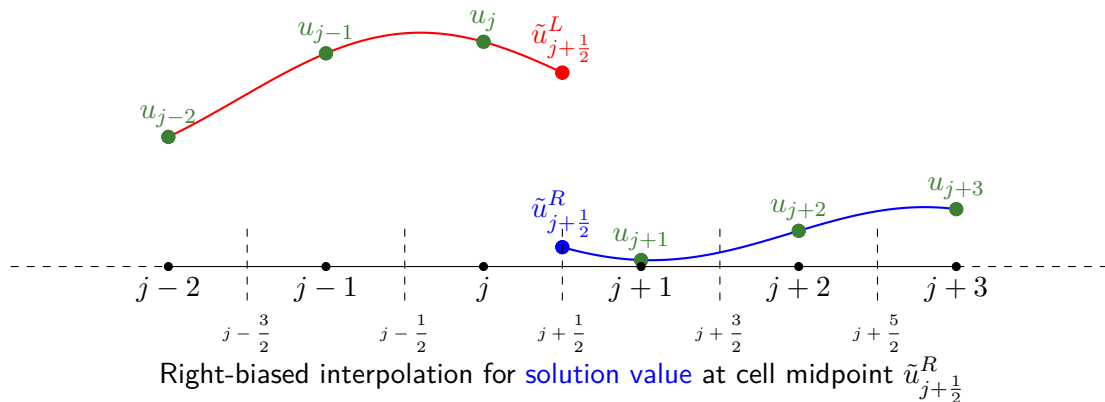


<sup>6</sup>Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

<sup>7</sup>Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".



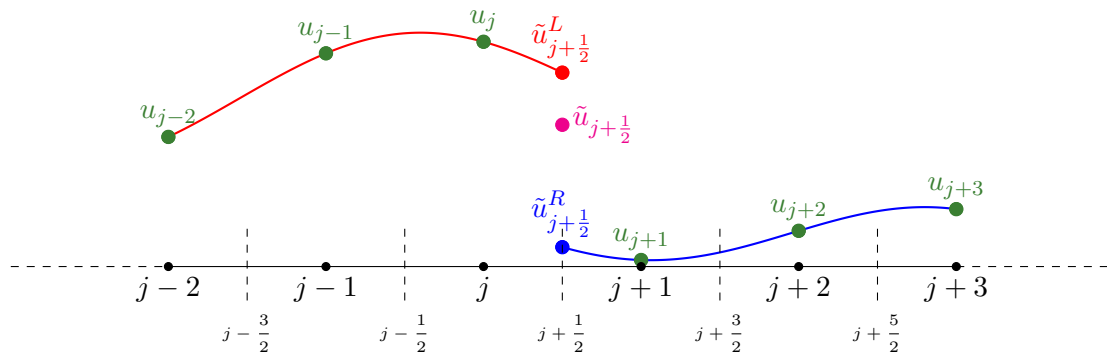
# Illustration of methodology of WCNS's <sup>6 7</sup>



<sup>6</sup>Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

<sup>7</sup>Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

# Illustration of methodology of WCNS's <sup>6 7</sup>

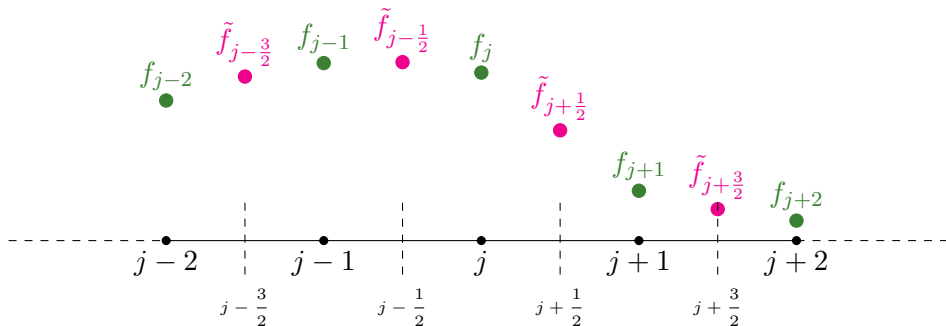


Flux-difference splitting method to get the **interface solution value and flux** at midpoint from left-biased and right-biased interpolated values

<sup>6</sup>Deng and Zhang, "Developing high-order weighted compact nonlinear schemes".

<sup>7</sup>Zhang, Jiang, and Shu, "Development of nonlinear weighted compact schemes with increasingly higher order accuracy".

# Illustration of methodology of WCNS's <sup>6 7</sup>

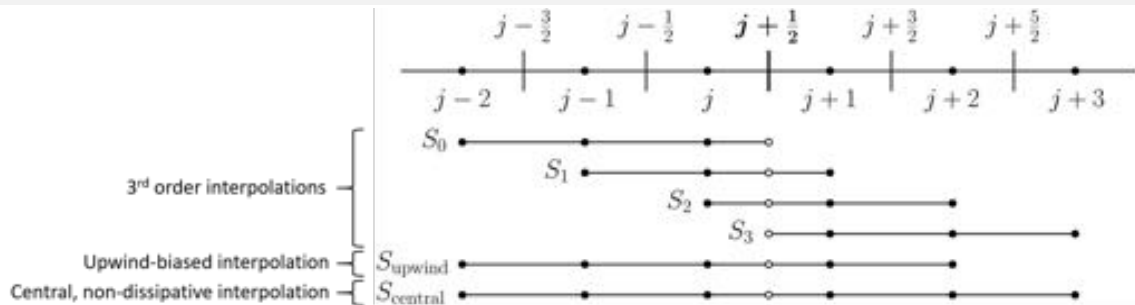


Explicit/compact finite difference to approximate  $\left. \frac{\partial f(u)}{\partial x} \right|_j$  at nodes, e.g.

explicit sixth order midpoint-and-node-to-node finite difference (MND):

$$\left. \frac{\partial f(u)}{\partial x} \right|_j \approx \frac{1}{\Delta x} \left[ \frac{3}{2} \left( \tilde{f}_{j+\frac{1}{2}} - \tilde{f}_{j-\frac{1}{2}} \right) - \frac{3}{10} (f_{j+1} - f_{j-1}) - \frac{25}{384} \left( \tilde{f}_{j+\frac{3}{2}} - \tilde{f}_{j-\frac{3}{2}} \right) \right]$$

# Left-biased explicit interpolations



$$EI_0 : \quad \tilde{u}_{j+\frac{1}{2}}^{(0)} = \frac{1}{8} (3u_{j-2} - 10u_{j-1} + 15u_j)$$

$$EI_1 : \quad \tilde{u}_{j+\frac{1}{2}}^{(1)} = \frac{1}{8} (-u_{j-1} + 6u_j + 3u_{j+1})$$

$$EI_2 : \quad \tilde{u}_{j+\frac{1}{2}}^{(2)} = \frac{1}{8} (3u_j + 6u_{j+1} - u_{j+2})$$

$$EI_3 : \quad \tilde{u}_{j+\frac{1}{2}}^{(3)} = \frac{1}{8} (15u_{j+1} - 10u_{j+2} + 3u_{j+3})$$

$$EI_{\text{upwind}} = \sum_k^2 d_k^{\text{upwind}} EI_k \quad (5^{\text{th}} \text{ order}); \quad EI_{\text{central}} = \sum_k^3 d_k^{\text{central}} EI_k \quad (6^{\text{th}} \text{ order})$$

# Nonlinear interpolations

In weighted essentially non-oscillatory (WENO) interpolations, the linear weights  $d_k$  are replaced with nonlinear weights  $\omega_k$  for shock-capturing:

$$EI_{\text{upwind}} = \sum_{k=0}^2 d_k^{\text{upwind}} EI_k \quad (5^{\text{th}} \text{ order}); \quad EI_{\text{central}} = \sum_{k=0}^3 d_k^{\text{central}} EI_k \quad (6^{\text{th}} \text{ order})$$

↓

$$EI_{\text{nonlinear}} = \sum_{k=0}^2 \omega_k^{\text{upwind}} EI_k \quad / \quad \sum_{k=0}^3 \omega_k^{\text{central}} EI_k$$

- $\omega_k^{\text{upwind}}$ : traditional WENO weights by Jiang and Shu (JS)<sup>8</sup> and improved weights (Z)<sup>9</sup>
- $\omega_k^{\text{central}}$ : CU-M2 weights<sup>10</sup>

<sup>8</sup>Guang-Shan Jiang and Chi-Wang Shu. "Efficient implementation of weighted ENO schemes". In: *Journal of computational physics* 126.1 (1996), pp. 202–228.

<sup>9</sup>Rafael Borges et al. "An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws". In: *Journal of Computational Physics* 227.6 (2008), pp. 3191–3211.

<sup>10</sup>XY Hu and Nikolaus A Adams. "Scale separation for implicit large eddy simulation". In: *Journal of Computational Physics* 230.19 (2011), pp. 7240–7249.

## Locally dissipative (LD) nonlinear weights

- The  $\text{LD}^{11}$  nonlinear weights (**hybrid weights**) are introduced for localized dissipation at shocks or discontinuities for regularization:

$$\omega_k = \begin{cases} \sigma \omega_k^{\text{upwind}} + (1 - \sigma) \omega_k^{\text{central}}, & \text{if } R_\tau > \alpha_{RL}^\tau \\ \omega_k^{\text{central}}, & \text{otherwise} \end{cases}, \quad k = 0, 1, 2, 3$$

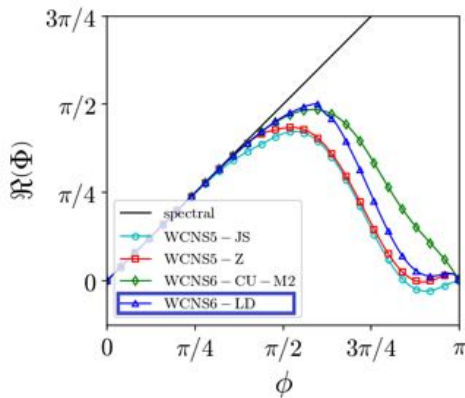
where  $R_\tau$  is a relative smoothness indicator.  $\sigma$  is a shock sensor.

- Ensure minimal numerical dissipation in smooth regions (central interpolation) and one-sided interpolation at discontinuities
- $\omega_k^{\text{upwind}}$  is the Z nonlinear weights and  $\omega_k^{\text{central}}$  is **improved** from CU-M2 nonlinear weights for localized numerical dissipation

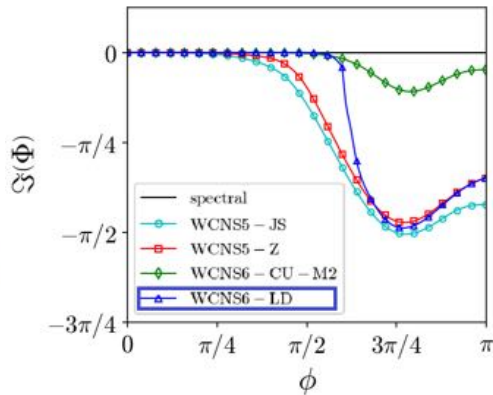
<sup>11</sup>Man Long Wong and Sanjiva K Lele. "High-order localized dissipation weighted compact nonlinear scheme for shock-and interface-capturing in compressible flows". In: *Journal of Computational Physics* 339 (2017), pp. 179–209.

## Approximate dispersion relation (ADR) technique<sup>12</sup>

- For linear schemes, analytical dispersion and dissipation characteristics can be obtained from Fourier analysis
- ADR used to compute the characteristics of the nonlinear schemes numerically:



(a) Dispersion characteristics

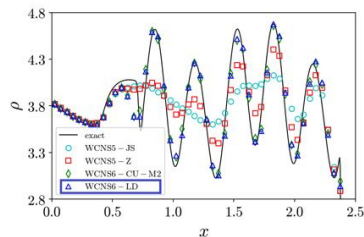
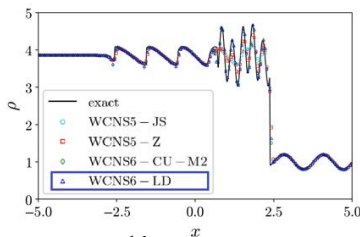


(b) Dissipation characteristics

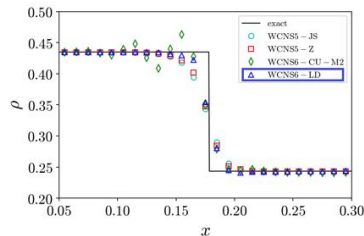
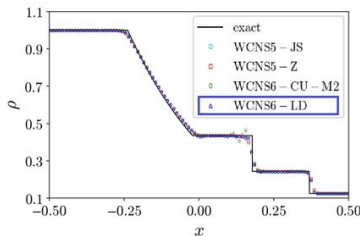
<sup>12</sup>Sergio Pirozzoli. "On the spectral properties of shock-capturing schemes". In: *Journal of Computational Physics* 219.2 (2006) pp. 489–497. [↗](#) [↖](#) [↕](#) [↔](#) [↻](#) [⌂](#)

# Numerical tests: 1D shock tube problems

1. Shu-Osher problem<sup>13</sup> [200 points]: Mach 3 shock interacting with a sinusoidal density field



2. Multi-species shock tube<sup>14</sup> [100 points]:

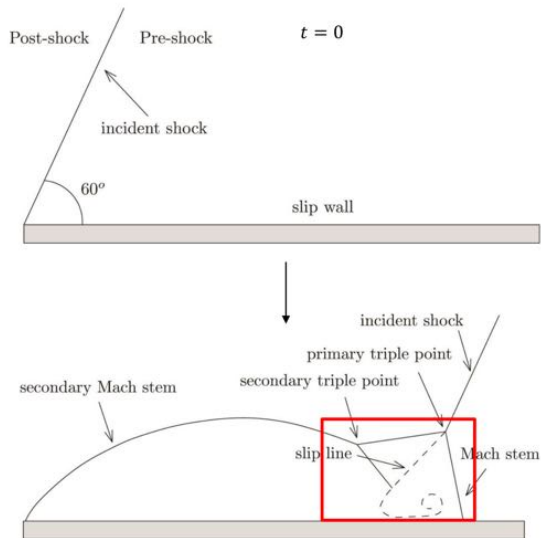


<sup>13</sup>Chi-Wang Shu and Stanley Osher. "Efficient implementation of essentially non-oscillatory shock-capturing schemes" In: *Journal of Computational Physics* 77.2 (1988), pp. 439–471



# Numerical test: 2D double Mach reflection<sup>15</sup>

- A Mach 10 shock impinges on the wall, and a complex shock reflection structure evolves
- Kelvin-Helmholtz instability along the slip line is only damped by numerical dissipation
- The smaller the numerical dissipation, the more the rolled up vortices along the slip line



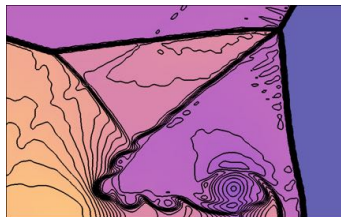
<sup>15</sup>Phillip Colella and Paul R Woodward. "The piecewise parabolic method (PPM) for gas-dynamical simulations". In: *Journal of computational physics* 54.1 (1984), pp. 174–201.

# Numerical test: 2D double Mach reflection (cont.)

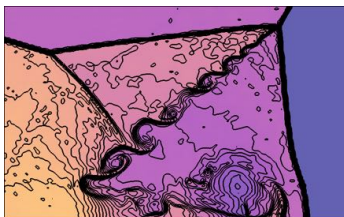
- Density contours [Full domain grid size:  $960 \times 240$ ]:



(a) WCNS5-JS



(b) WCNS5-Z



(c) WCNS6-CU-M2

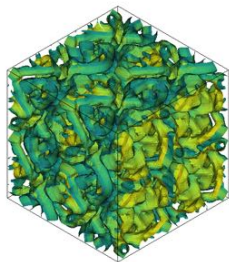


(d) WCNS6-LD

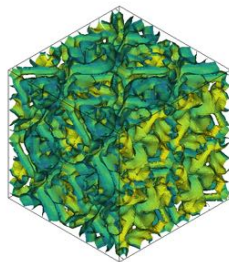
- WCNS5-JS and WCNS5-Z too dissipative to produce rolled-up vortices along the slip line
- WCNS6-CU-M2 and WCNS6-LD can capture much more fine-scale vortical structures along the slip line

# Numerical test: 3D Taylor-Green vortex

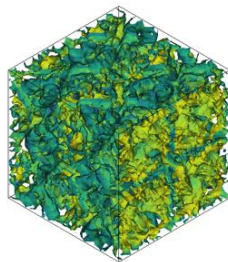
- An essentially incompressible periodic problem
- As time evolves, the inviscid vortex stretches and produces features at smaller scales
- Zero Q-criterion at  $t = 8$  with  $64^3$  grid:



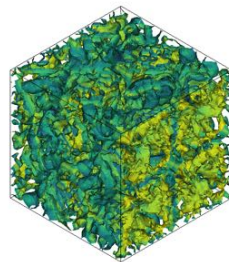
(a) WCNS5-JS



(b) WCNS5-Z



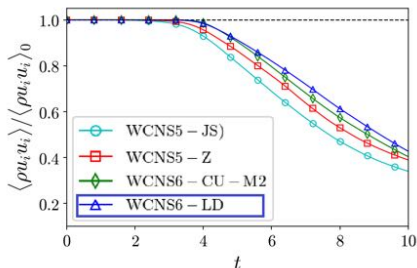
(c) WCNS6-CU-M2



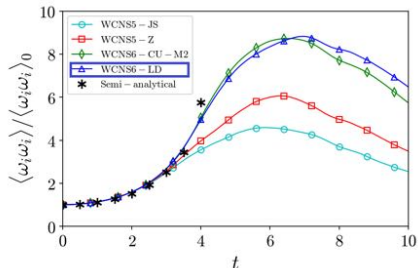
(d) WCNS6-LD

- Finer features are captured with WCNS6-CU-M2 and WCNS6-LD

# Numerical test: 3D Taylor-Green vortex (cont.)

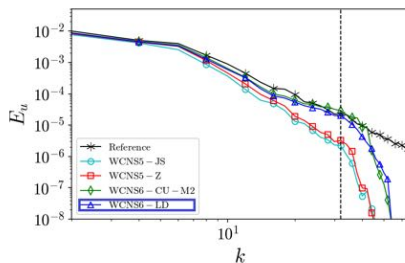


(a) Kinetic energy



(b) Enstrophy

Spectra of  $u$  at  $t = 5$ :



- **WCNS6-LD** preserves more KE over times
- Both WCNS6's outperform WCNS5's in predicting growth of enstrophy
- Both WCNS6's can better capture features up to high wavenumber

# Summary

- Improved nonlinear interpolation developed for a type of nonlinear schemes for problems with shocks and material interfaces
- The interpolation adaptively switches between one-sided interpolation around discontinuities and non-dissipative central interpolation in smooth regions
- The improved scheme WCNS-LD:
  - robust at shocks and discontinuities through the regularization
  - good resolution and low dissipation properties that are more suited for vortical features

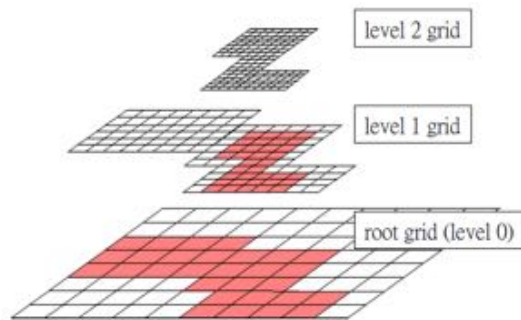
# Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows
2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability
3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock
4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability

# Overview of patch-based adaptive mesh refinement (AMR)

- Patch-based AMR<sup>1617</sup> designed for uniform structured Cartesian grids
- A hierarchy of nested "patches" of levels of varying grid resolution
- **Multi-time stepping** with Runge-Kutta schemes:

$$\frac{\Delta t_l}{\Delta x_l} = \frac{\Delta t_{l-1}}{\Delta x_{l-1}} = \dots = \frac{\Delta t_0}{\Delta x_0}$$



- Requires numerical scheme in **conservative** form for treatment at coarse-fine AMR grid boundaries to ensure **discrete conservation**:

$$\frac{\partial u_{i,j}}{\partial t} + \frac{\hat{F}_{i+\frac{1}{2},j} - \hat{F}_{i-\frac{1}{2},j}}{\Delta x} + \frac{\hat{G}_{i,j+\frac{1}{2}} - \hat{G}_{i,j-\frac{1}{2}}}{\Delta y} = 0$$

<sup>16</sup>Marsha J Berger and Phillip Colella. "Local adaptive mesh refinement for shock hydrodynamics". In: *Journal of computational Physics* 82.1 (1989), pp. 64–84.

<sup>17</sup>Marsha J Berger and Joseph Oliger. "Adaptive mesh refinement for hyperbolic partial differential equations". In: *Journal of computational Physics* 53.3 (1984), pp. 484–512.

# Relation between finite difference schemes and flux difference form<sup>18</sup>

- For a central finite difference scheme (compact or explicit) for flux derivative:

$$\alpha \hat{F}'_{j-1} + \beta \hat{F}'_j + \alpha \hat{F}'_{j+1} = \frac{1}{\Delta x} \left( -a_{\frac{5}{2}} F_{j-2} - a_2 F_{j-\frac{3}{2}} - a_{\frac{3}{2}} F_{j-1} - a_1 F_{j-\frac{1}{2}} + a_1 F_{j+\frac{1}{2}} + a_{\frac{3}{2}} F_{j+1} + a_2 F_{j+\frac{3}{2}} + a_{\frac{5}{2}} F_{j+2} \right)$$

- Can be rewritten into flux difference form:

$$\alpha \hat{F}_{j-\frac{1}{2}} + \beta \hat{F}_{j+\frac{1}{2}} + \alpha \hat{F}_{j+\frac{3}{2}} = a_{\frac{5}{2}} F_{j-1} + a_2 F_{j-\frac{1}{2}} + \left( a_{\frac{3}{2}} + a_{\frac{5}{2}} \right) F_j + (a_1 + a_2) F_{j+\frac{1}{2}} + \left( a_{\frac{3}{2}} + a_{\frac{5}{2}} \right) F_{j+1} + a_2 F_{j+\frac{3}{2}} + a_{\frac{5}{2}} F_{j+2}$$

s.t.

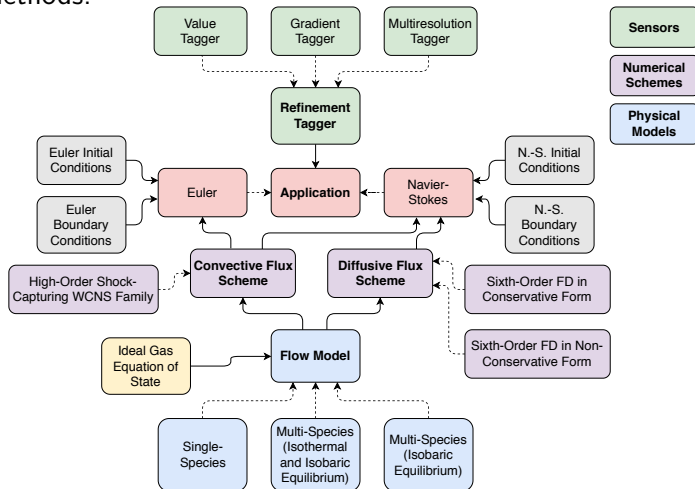
$$\boxed{\hat{F}'_j = \frac{1}{\Delta x} \left( \hat{F}_{j+\frac{1}{2}} - \hat{F}_{j-\frac{1}{2}} \right)}$$

<sup>18</sup> A Subramaniam, ML Wong, and SK Lele. "A High-Order Weighted Compact High Resolution Scheme with Boundary Closures for Compressible Turbulent Flows with Shocks". In: *arXiv preprint arXiv:1809.05784* (2018).



# Hydrodynamics Adaptive Mesh Refinement Simulator (HAMeRS)<sup>19</sup>

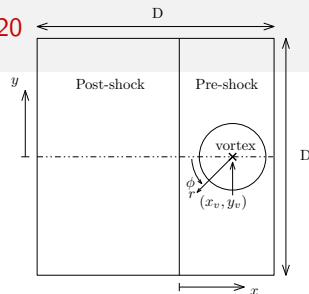
In-house flow solver built on parallel SAMRAI library from LLNL to simulate compressible single-species and multi-species flows with adaptive mesh refinement (AMR) and high-order shock-capturing methods:



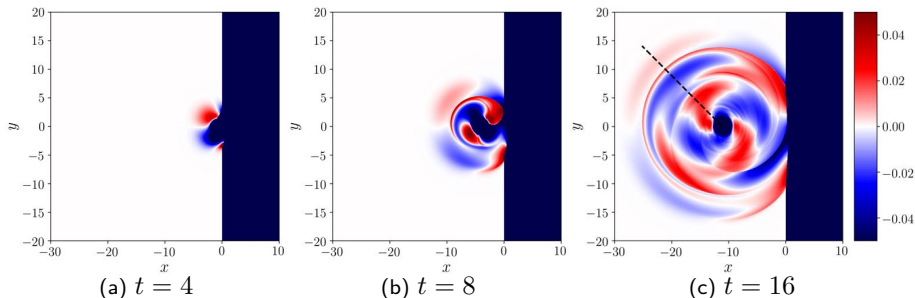
<sup>19</sup>Man Long Wong. Hydrodynamics Adaptive Mesh Refinement Simulator. <https://github.com/mlwong/HAMeRS>. 2018.

# Numerical test: 2D inviscid shock-vortex interaction<sup>20</sup>

- Isentropic vortex interacts with Mach 1.2 stationary shock
- Distorted vortex produces reflected shocks
- Multiple sound waves generated from reflected shock-vortex interaction



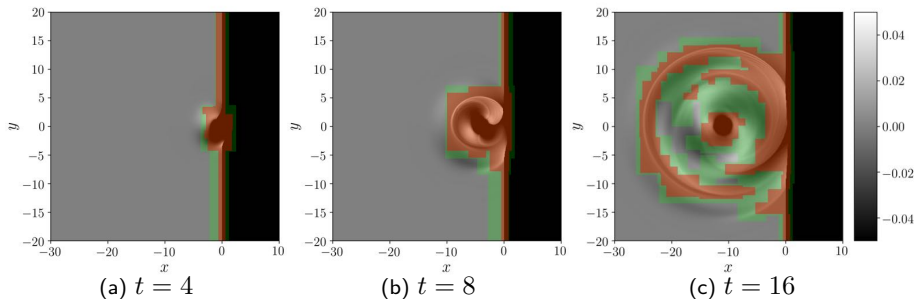
Sound pressure,  $(p - p_\infty) / (\rho_\infty c_\infty^2)$ , of reference solution with grid resolution  $4096 \times 4096$ :



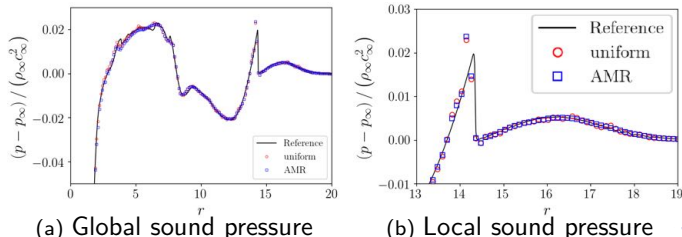
<sup>20</sup>Osamu Inoue and Yuji Hattori. "Sound generation by shock-vortex interactions". In: *Journal of Fluid Mechanics* 380 (1999), pp. 81–116.

# Numerical test: 2D inviscid shock-vortex interaction (cont.)

Refined regions of AMR simulation with base grid resolution  $128 \times 128$  and 1 : 2 refinement ratio (green: level 1; red: level 2):



Comparison with  $512 \times 512$  uniform grid simulation:



# Numerical test: 2D inviscid shock-vortex interaction (cont.)

- Weighted number of cells:

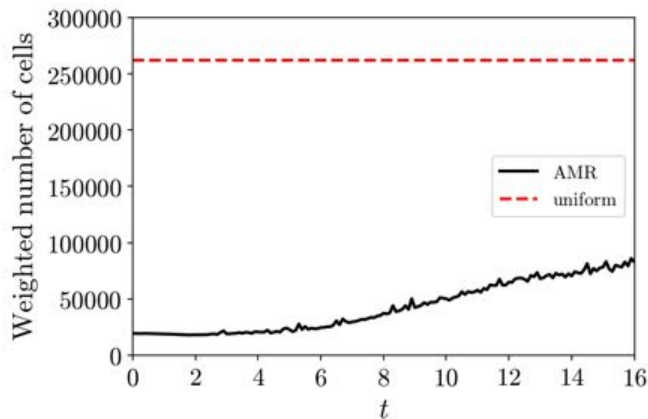
$$\sum_{l=0}^{l_{max}} \omega_l N_l, \quad \omega_l = \frac{\Delta x_{l_{max}}}{\Delta x_l}$$

- In this test problem:

$$\omega_0 = 1/4,$$

$$\omega_1 = 1/2,$$

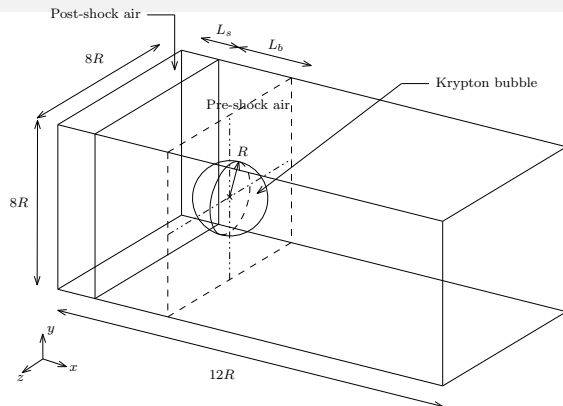
$$\omega_2 = 1$$



Weighted number of cells of AMR simulation  $\approx 30\%$  of number of cells of uniform grid (262144 cells) simulation at the end

# Numerical test: 3D viscous shock-bubble interaction

- $Ma_s = 1.68$ ,  $R = 1.016$  mm
- Material interface with characteristic length scale  $\epsilon_i = 0.125$  mm
- A quadrant of the domain is simulated



- Different grids settings:

Grid	Base grid resolution	Refinement ratios	Finest grid spacing ( $\mu\text{m}$ )
A	$384 \times 128 \times 128$	1:2, 1:2	7.94
B	$768 \times 256 \times 256$	1:2, 1:2	3.97
C	$1536 \times 512 \times 512$	1:2, 1:2	1.98

- Gradient sensor on pressure, multiresolution sensor on density, and sensor on mass fraction used for refinement

## Numerical test: 3D viscous shock-bubble interaction (cont.)

- Conservative multi-component Navier-Stokes equations for ideal fluid mixture are solved:

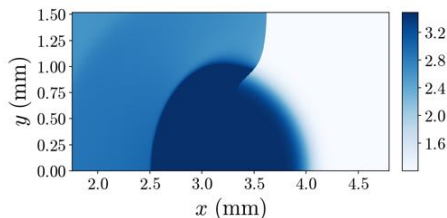
$$\begin{aligned}\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) + \nabla \cdot \mathbf{J}_i &= 0 \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \boldsymbol{\delta} - \boldsymbol{\tau}) &= 0 \\ \frac{\partial E}{\partial t} + \nabla \cdot [(E + p) \mathbf{u}] - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u} - \mathbf{q}_c - \mathbf{q}_d) &= 0\end{aligned}$$

where  $\rho$ ,  $\mathbf{u}$ ,  $p$  and  $E$  are the density, velocity vector, pressure and total energy of the fluid mixture respectively.  $Y_i$  is the mass fraction of species  $i = 1, 2, \dots, N$ , with  $N$  the total number of species.

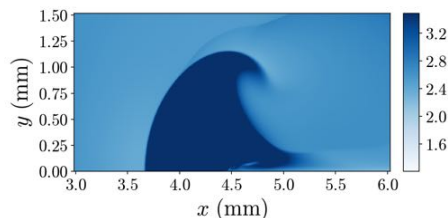
- $\mathbf{J}_i$  is diffusive mass flux for each species.  $\boldsymbol{\tau}$ ,  $\mathbf{q}_c$  and  $\mathbf{q}_d$  are viscous stress tensor, conductive heat flux and inter-species diffusional enthalpy flux respectively of the mixture.
- Sixth order finite differences for viscous and diffusive fluxes

## Numerical test: 3D viscous shock-bubble interaction (cont.)

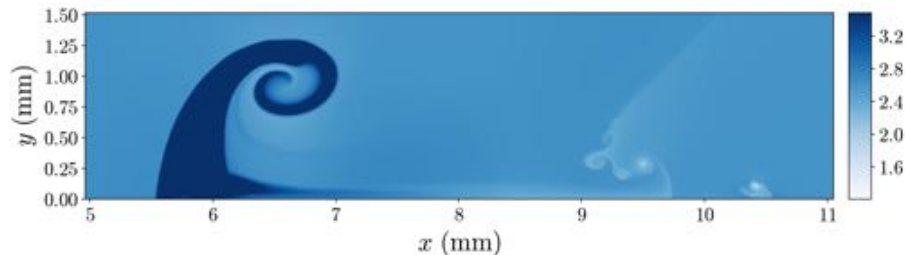
- Density fields in  $xy$  plane at  $z = 0$  of AMR simulation with grid C:



(a)  $t = 2.8 \mu\text{s}$



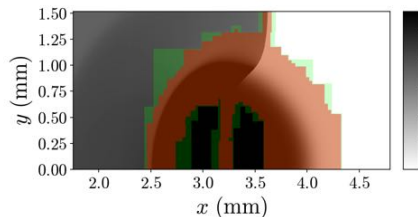
(b)  $t = 8.8 \mu\text{s}$



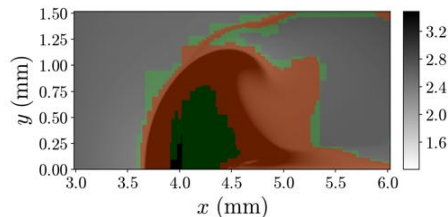
(c)  $t = 17.6 \mu\text{s}$

# Numerical test: 3D viscous shock-bubble interaction (cont.)

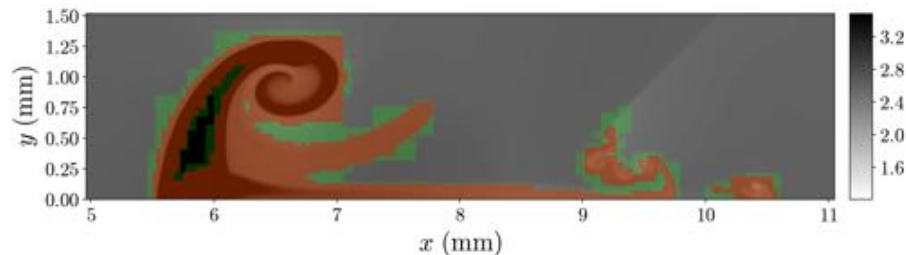
- Refined regions (green: level 1; red: level 2):



(a)  $t = 2.8 \mu\text{s}$



(b)  $t = 8.8 \mu\text{s}$

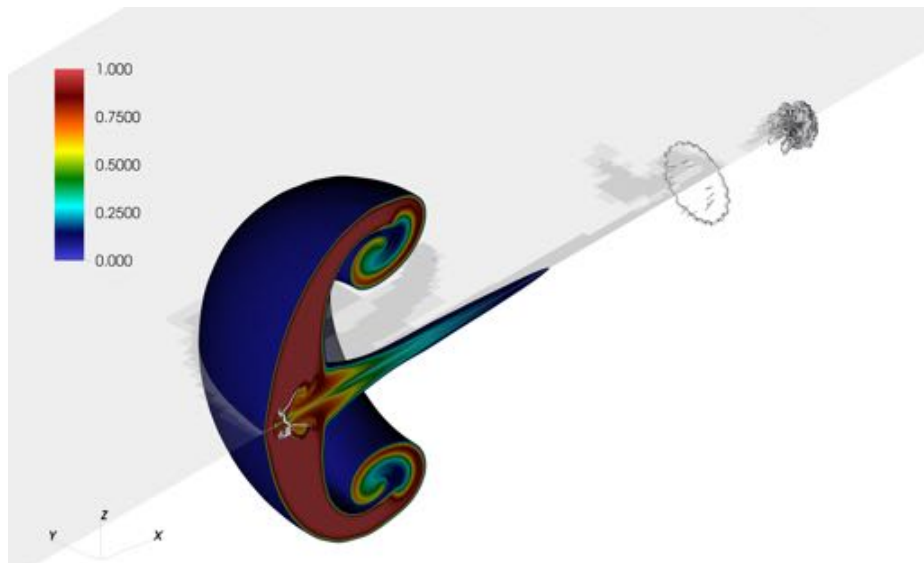


(c)  $t = 17.6 \mu\text{s}$

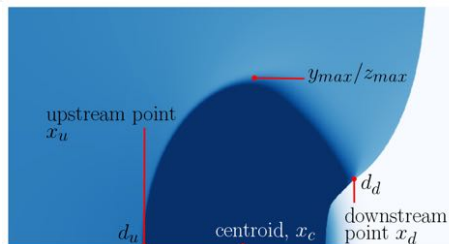


## Numerical test: 3D viscous shock-bubble interaction (cont.)

3D visualization of mass fraction with grid C at end of simulation  $t = 17.6 \mu s$



# Numerical test: 3D viscous shock-bubble interaction (cont.)

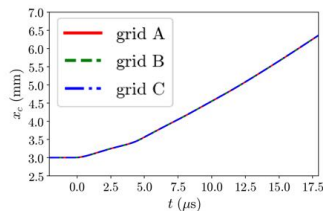


- $y_{max}$  is  $y$  coordinate of the upper point with  $SF_6$  concentration equals  $0.01 \max(Y_{SF6})$

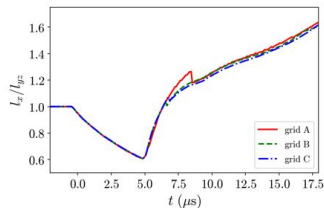
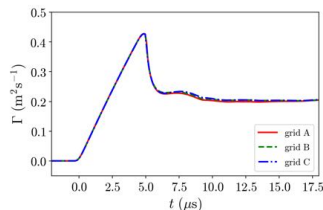
$$l_x = x_d - x_u$$

$$l_{yz} = y_{max} + z_{max}$$

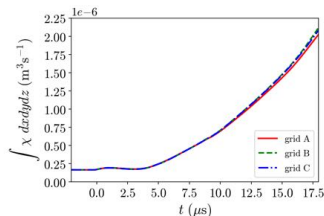
- All statistical quantities of interests are grid converged



(a) Centroid

(b)  $l_x/l_y$ 

(c) Circulation



(d) Integrated scalar dissipation rate

# Summary

- AMR framework developed for multi-species CFD applications
- Physics-based sensors such as gradient and multiresolution sensors implemented to detect features for refinement
- Framework successfully tested with simulations<sup>21</sup> that consist of interactions between shocks, material interfaces, and vortices
- The sensors for mesh refinement can successfully identify:
  - Shock wave and acoustic waves
  - Vortical features
  - Mixing regions

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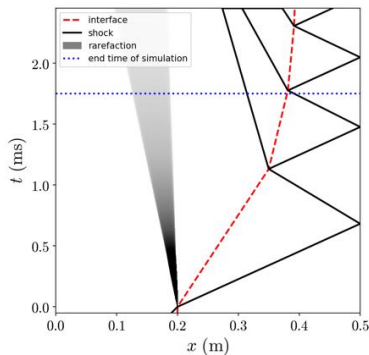
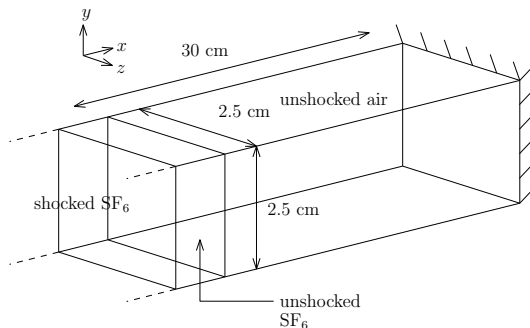
<sup>21</sup>One more 2D viscous shock-cylinder interaction problem is presented in thesis

# Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows
2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability
3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock
4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability

## Problem setup

- Compressible 2D and 3D multi-species Navier-Stokes simulations set up to study shock-induced mixing between  $\text{SF}_6$  and air due to RM instability:



- $Ma_s = 1.45$  (a) 3D configuration

- $At = \frac{\rho_{\text{SF}_6} - \rho_{\text{air}}}{\rho_{\text{SF}_6} + \rho_{\text{air}}} = 0.68$

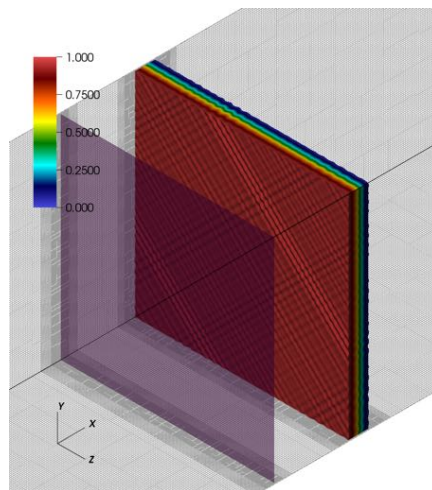
- 2D domain is cross-section of the 3D domain
- Mixing region shocked **twice** (first shock and re-shock)

(b) Space-time ( $x$ - $t$ ) diagram

# Perturbations

Perturbation modes seeded on the interfaces:

- 2D:
 
$$S(y) = A \sum_m \cos \left( \frac{2\pi m}{L_y} y + \phi_m \right)$$
- 3D:
 
$$S(y, z) = A \sum_m \cos \left( \frac{2\pi m}{L_{yz}} y + \phi_m \right) \cos \left( \frac{2\pi m}{L_{yz}} z + \psi_m \right)$$
- 11 modes in total:  $0.833 \text{ mm} \leq \lambda_m \leq 1.25 \text{ mm}$
- $A = 0.0141 \text{ mm}$
- Estimated with impulsive theory, 2D and 3D problems have same:
  - linear growth rates  $\dot{\eta}_{imp}$
  - time scales  $\tau_c$



initial conditions

# Configurations of 2D and 3D adaptive mesh refinement (AMR) simulations

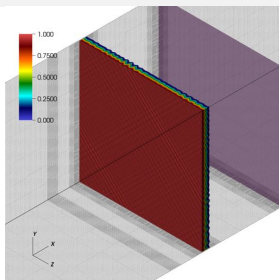
- Simulated with the AMR solver (HAMeRS)
- Sixth order WCNS-LD for convective flux
- Sixth order finite differences for diffusive and viscous fluxes
- Three levels of adaptive meshes (two levels of AMR)
- Gradient and multiresolution sensors; also sensor on mass fraction field
- Grid resolutions used for convergence test:

2D Grid	Base Grid Resolution	Refinement Ratio	Finest Grid Spacing (mm)
D	$2560 \times 128$	1:2, 1:4	0.0244
E	$5120 \times 256$	1:2, 1:4	0.0122
F	$10240 \times 512$	1:2, 1:4	0.0061
G	$20480 \times 1024$	1:2, 1:4	0.0031

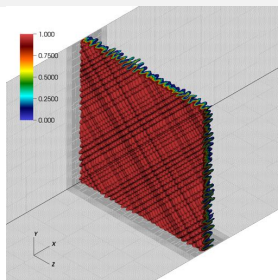
3D Grid	Base Grid Resolution	Refinement Ratio	Finest Grid Spacing (mm)	Maximum Weighted Number of Cells
B	$640 \times 32 \times 32$	1:2, 1:4	0.0977	30M
C	$1280 \times 64 \times 64$	1:2, 1:4	0.0488	144M
D	$2560 \times 128 \times 128$	1:2, 1:4	0.0244	778M

- $\sim 34$  points across smallest initial wavelength for grid D

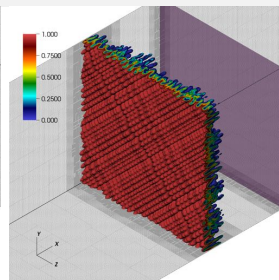
# Visualizations of mole fraction (3D, grid D)



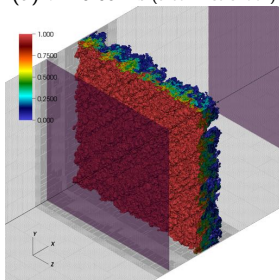
(a)  $t = 0.05$  ms (after first shock)



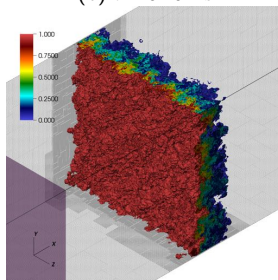
(b)  $t = 0.40$  ms



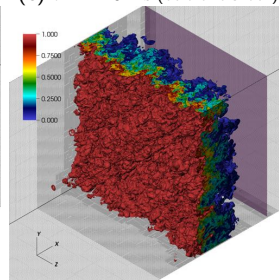
(c)  $t = 1.10$  ms (before re-shock)



(d)  $t = 1.20$  ms (after re-shock)



(e)  $t = 1.40$  ms

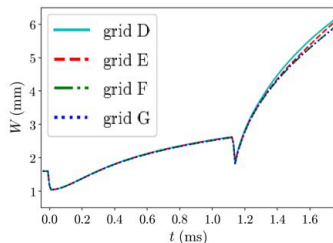


(f)  $t = 1.75$  ms

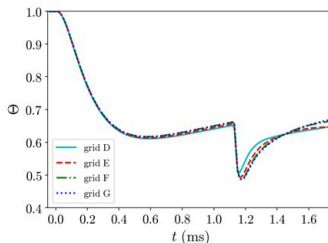


## 2D grid convergence study (over 24 realizations)

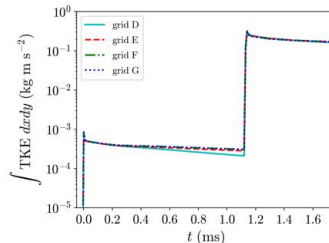
$$\text{Mixing width } W = \int 4\bar{X}_{SF6}(1 - \bar{X}_{SF6})dx; \quad \text{Mixedness } \Theta = \frac{\int \overline{X_{SF6}(1 - X_{SF6})}dx}{\int \bar{X}_{SF6}(1 - \bar{X}_{SF6})dx}; \quad \text{TKE} = \frac{1}{2}\rho u_i'' u_i''$$



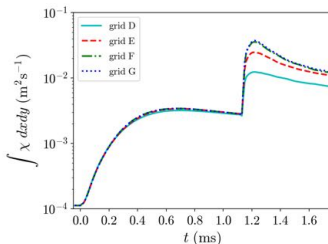
(a) Mixing width



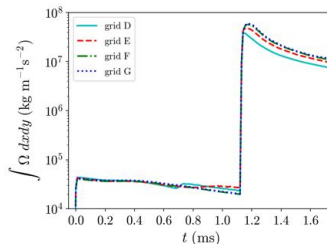
(b) Mixedness



(c) TKE (integrated)



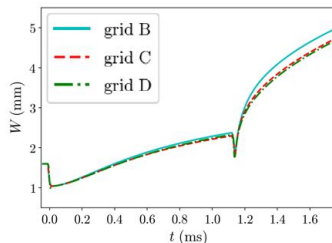
(d) Scalar dissipation rate (integrated)



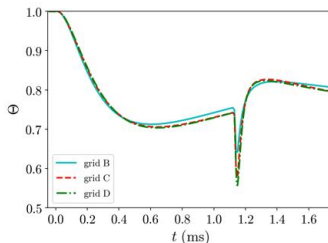
(e) Enstrophy (integrated)

# 3D grid convergence study

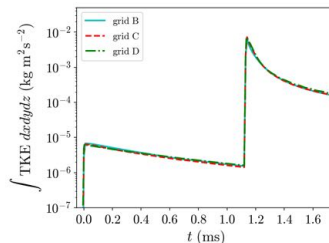
$$\text{Mixing width } W = \int 4\bar{X}_{SF6}(1 - \bar{X}_{SF6})dx; \quad \text{Mixedness } \Theta = \frac{\int \overline{X_{SF6}(1 - X_{SF6})}dx}{\int \bar{X}_{SF6}(1 - \bar{X}_{SF6})dx}; \quad \text{TKE} = \frac{1}{2}\rho u_i'' u_i''$$



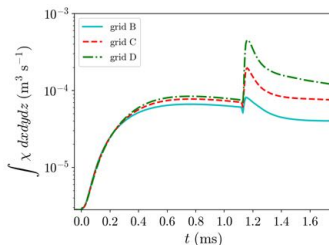
(a) Mixing width



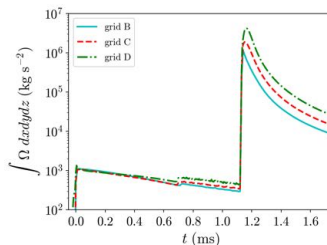
(b) Mixedness



(c) TKE (integrated)

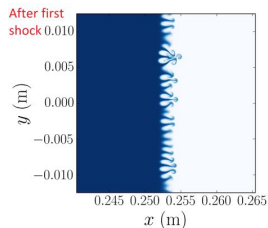
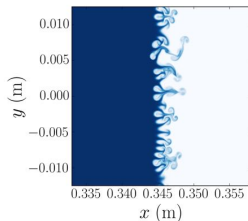
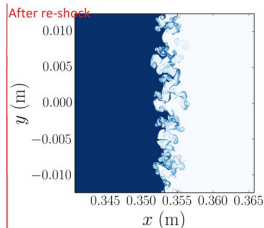
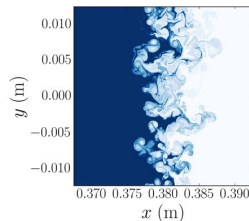


(d) Scalar dissipation rate (integrated)

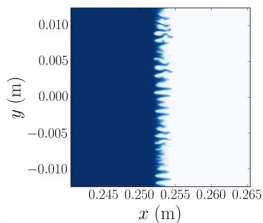
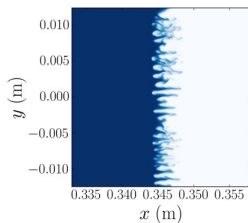
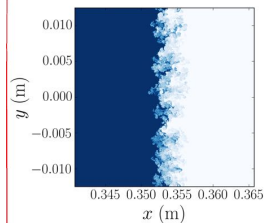
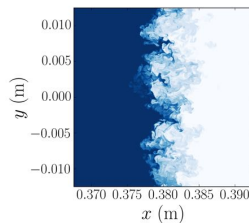


(e) Enstrophy (integrated)

# Mole fraction fields $t^* = t/\tau_c$

(a)  $t^* = 7.5$  ( $t = 0.40$  ms)(b)  $t^* = 20.7$  ( $t = 1.10$  ms)(c)  $t^* = 22.6$  ( $t = 1.20$  ms)(d)  $t^* = 32.9$  ( $t = 1.75$  ms)

## 2D, grid G

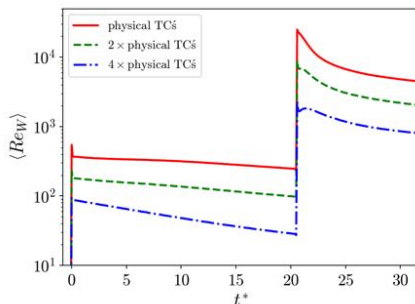
(a)  $t^* = 7.5$  ( $t = 0.40$  ms)(b)  $t^* = 20.7$  ( $t = 1.10$  ms)(c)  $t^* = 22.6$  ( $t = 1.20$  ms)(d)  $t^* = 32.9$  ( $t = 1.75$  ms)

## 3D, grid D

## Reduced Reynolds number 3D simulations

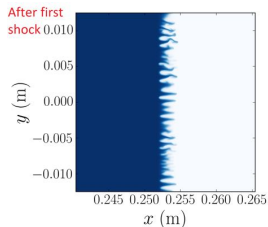
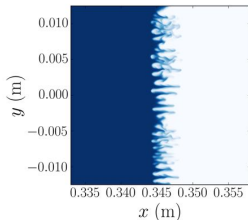
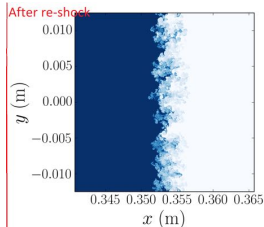
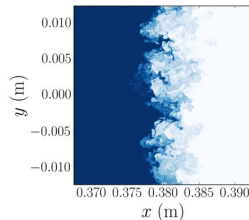
- Reynolds number  $Re_W$  is reduced by increasing physical transport coefficients (TC's) by factors of 2 & 4 ( $\mu$ ,  $\mu_v$ ,  $D$ , and  $\kappa$ ). This is as same as cases with reduced  $Re_W$ , while  $Sc$  and  $Pr$  unchanged.

$$Re_W = \frac{\bar{\rho} u_{rms} W}{\bar{\mu}}, \quad \text{where } u_{rms} = \sqrt{u_i'' u_i'' / 3}$$

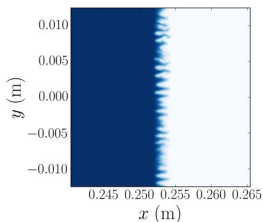
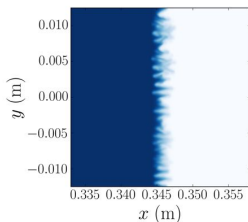
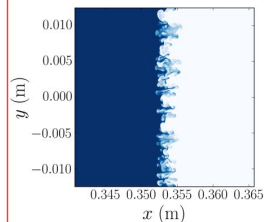
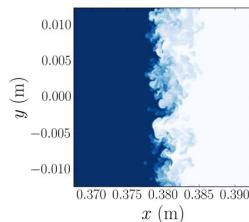


- $\langle \cdot \rangle$  is additional averaging in central part of mixing layer:  $4\bar{X}_{SF_6}(1 - \bar{X}_{SF_6}) > 0.9$

# Mole fraction fields

(a)  $t^* = 7.5$  ( $t = 0.40$  ms)(b)  $t^* = 20.7$  ( $t = 1.10$  ms)(c)  $t^* = 22.6$  ( $t = 1.20$  ms)(d)  $t^* = 32.9$  ( $t = 1.75$  ms)

## Physical transport coefficients, grid D

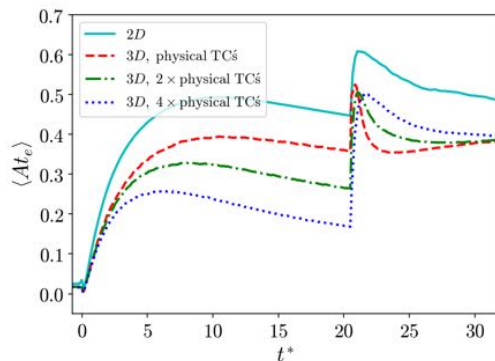
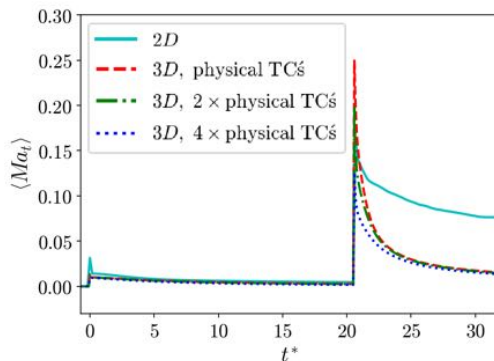
(a)  $t^* = 7.5$  ( $t = 0.40$  ms)(b)  $t^* = 20.7$  ( $t = 1.10$  ms)(c)  $t^* = 22.6$  ( $t = 1.20$  ms)(d)  $t^* = 32.9$  ( $t = 1.75$  ms)

## 4× physical transport coefficients, grid D

# Flow compressibility and effective Atwood number

- Turbulent Mach number  $Ma_t$  and effective Atwood number  $At_e$ :

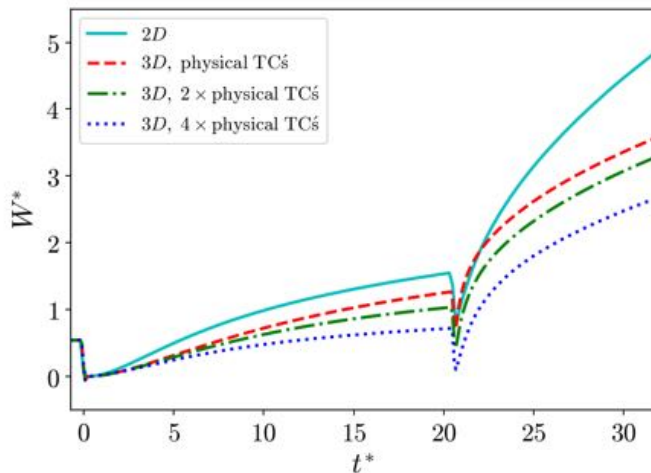
$$Ma_t = \frac{\sqrt{3}u_{rms}}{\bar{c}}, \quad At_e = \frac{\sqrt{\rho'^2}}{\bar{\rho}}$$



- Flows are weakly compressible
- $At_e \approx 0$  due to initially diffuse interface, but flows become non-Boussinesq ( $At_e > 0.05$ ) as the interfaces become sharper after first shock and re-shock

## Mixing: mixing width

- The mixing width is normalized by  $\dot{\eta}_{imp}$  and  $\tau_c$ : 
$$W^* = \frac{W - W|_{t=0}}{\dot{\eta}_{imp}\tau_c}$$
- With physical TC's,  $W^*$  of 2D case grows at a faster rate compared to that of 3D case after first shock initially but growth rates are similar at late times
- After re-shock, the 2D mixing width grows at a much faster rate
- 3D case with reduced Reynolds number has slower growth rate in mixing width before re-shock but growth rates are similar after re-shock

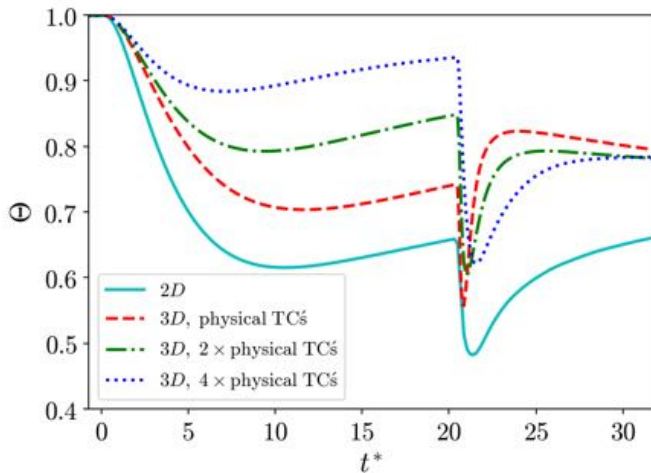


## Mixing: mixedness

- The mixedness is defined as:

$$\Theta = \frac{\int \bar{X}_{\text{SF}_6} (1 - \bar{X}_{\text{SF}_6}) dx}{\int \bar{X}_{\text{SF}_6} (1 - \bar{X}_{\text{SF}_6}) dx}$$

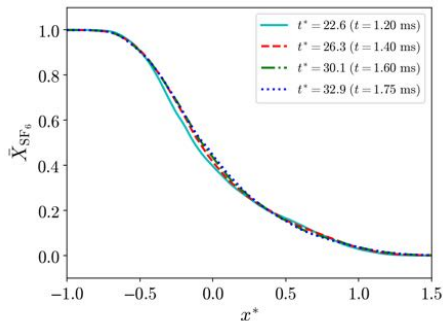
- Mixedness quantifies the amount of fluids molecularly mixed within the mixing region
- The 2D and 3D mixedness values are converging to 0.7 and 0.8 respectively [0.85 for 3D RMI from Tritschler et al.<sup>22</sup>, 0.8 for 3D RMI from Mohaghar et al.<sup>23</sup>]



<sup>22</sup>Tritschler et al., "On the Richtmyer–Meshkov instability evolving from a deterministic multimode planar interface".

<sup>23</sup>Mohaghar et al., "Evaluation of turbulent mixing transition in a shock-driven variable-density flow".





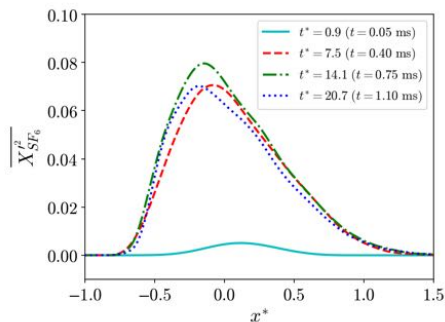
(b) After reshock, 3D

- The normalized position is defined as:  $x^* = \frac{x - x_i}{W(t)}$
- Asymmetric, spikes penetrate more than bubbles
- Profiles collapse quite well at late times, similar to planar Rayleigh-Taylor instability<sup>24</sup>

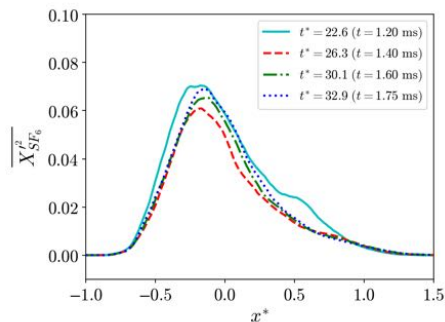
<sup>24</sup>Daniel Livescu et al. "High-Reynolds number Rayleigh–Taylor turbulence". In: *Journal of Turbulence* 10 (2009), N13.        

## Mixing: mole fraction variance profiles

$$\bullet \Theta = \frac{\int \overline{X_{\text{SF}_6}} (1 - \overline{X_{\text{SF}_6}}) dx}{\int \bar{X}_{\text{SF}_6} (1 - \bar{X}_{\text{SF}_6}) dx} = 1 - 4 \int \overline{X_{\text{SF}_6}'^2} dx^*$$



(a) After first shock, before reshock, 3D



(b) After reshock, 3D

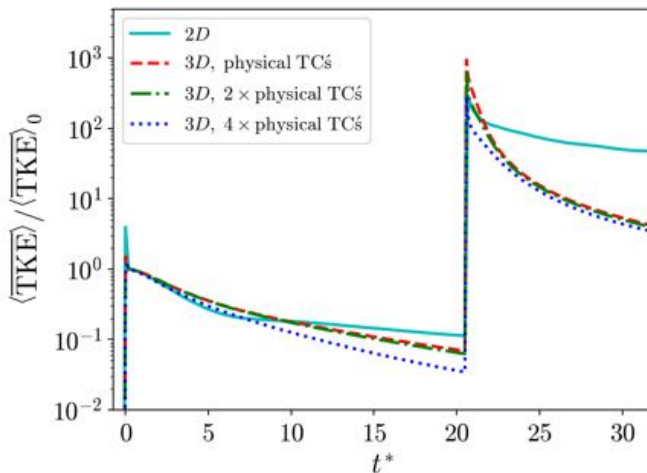
- Fluids harder to mix in the heavier fluid side indicated by larger variance
- Approaching self-similarity near end of simulations

# TKE time evolution

- TKE is defined as:

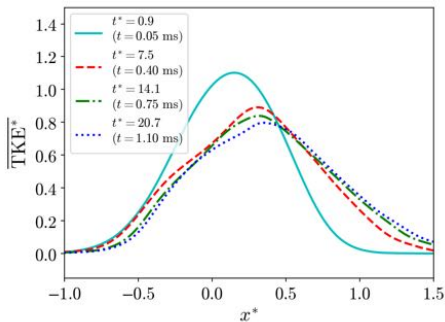
$$\text{TKE} = \frac{1}{2} \rho u_i'' u_i''$$

- TKE decays at faster rate for 3D problem compared to 2D
- Among 3D cases, TKE decays at faster rate before re-shock for case with smaller Reynolds number
- After re-shock, all 3D cases have similar TKE decay rates

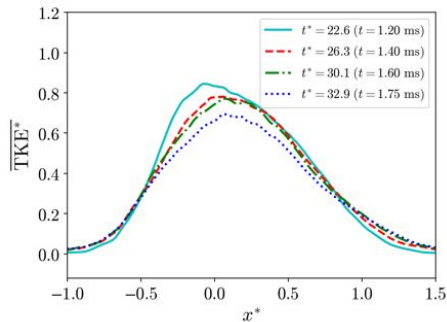


# Turbulent kinetic energy (TKE) profiles

- The TKE is normalized as: 
$$\text{TKE}^* = \frac{(\text{TKE}) W}{\int \overline{\text{TKE}} dx}$$



(a) After first shock, before reshock, 3D



(b) After reshock, 3D

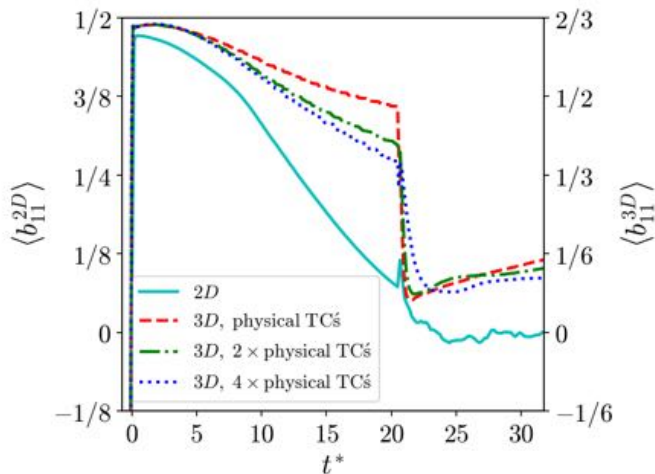
- Peak of TKE is biased towards the lighter fluid side, especially before re-shock

## Anisotropy

- The Reynolds stress anisotropy tensor  $b_{ij}$  for 2D and 3D flows defined as:

$$b_{ij}^{2D} = \frac{\tilde{R}_{ij}}{\tilde{R}_{kk}} - \frac{1}{2}\delta_{ij}, \quad b_{ij}^{3D} = \frac{\tilde{R}_{ij}}{\tilde{R}_{kk}} - \frac{1}{3}\delta_{ij}, \quad \text{where } \tilde{R}_{ij} = \frac{\overline{\rho u_i'' u_j''}}{\bar{\rho}}$$

- 2D Reynolds normal stresses becoming isotropic at a faster rate than 3D stresses before re-shock
- After re-shock, 2D Reynolds normal stresses become isotropic



# Summary

- 2D and 3D RMI have very different time evolution for mixing width and TKE and final mixedness values
  - Reynolds stresses of 2D flow approaching isotropy quickly after both shocks; Reynolds stresses of 3D flows remain anisotropic at the of simulations
  - Fluids are more difficult to mix in 2D configuration
- 
- Reducing  $Re_W$  has significant effect before re-shock:
    - smaller growth rate of  $W$
    - larger  $\Theta$
    - larger decay rate of TKE
  - Reynolds number has much smaller effect on the growth of mixing width/decay of TKE after re-shock

More analysis on probability density functions and spectra can be found in manuscript submitted to Physical Review Fluids<sup>25</sup>

<sup>25</sup>Man Long Wong, Daniel Livescu, and Sanjiva K. Lele. "High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock". In: *arXiv preprint arXiv:1812.01785* (2018).

# Outline

1. A localized dissipation nonlinear scheme for shock- and interface-capturing in compressible flows
2. An adaptive mesh refinement framework for multi-species simulations with shock-capturing capability
3. High-resolution Navier-Stokes simulations of Richtmyer-Meshkov instability with re-shock
4. Budget of turbulent mass flux and its closure for Richtmyer-Meshkov instability

# Favre-averaged momentum equation

- Direct numerical simulation (DNS) or large eddy simulation (LES) still very expensive
- Reynolds-averaged / Favre-averaged Navier-Stokes (RANS/FANS) simulation with **turbulence modeling** is an interim tool
- Most turbulent mixing models **only tested with experimental results** for RM turbulence
- **High-fidelity simulation data** also important for model validation
- Favre-averaged momentum equation ( $\tilde{\cdot} = \overline{\rho(\cdot)}/\bar{\rho}$ ):

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_k \tilde{u}_i)}{\partial x_k} = - \frac{\partial (\bar{p} \delta_{ki})}{\partial x_k} + \frac{\partial \bar{\tau}_{ki}}{\partial x_k} - \frac{\partial (\bar{\rho} \tilde{R}_{ki})}{\partial x_k}$$

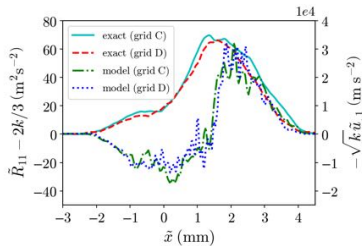
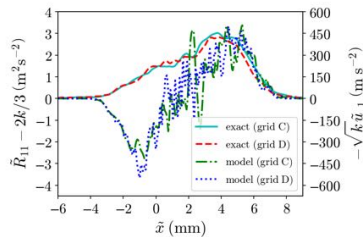
- $\tilde{R}_{ij} = \overline{\rho u_i'' u_j''} / \bar{\rho}$ : Favre-averaged Reynolds stress



## Reynolds stress

- Algebraic closure model based on turbulent kinetic energy is not good:

$$\tilde{R}_{ij} \approx \frac{2}{3}k\delta_{ij} - 2C_\mu S\sqrt{k}\tilde{S}_{ij}, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij},$$

(a)  $t = 1.20$  ms(b)  $t = 1.75$  ms

- To improve, transport equation of  $\tilde{R}_{ij}$  is considered:

$$\underbrace{\frac{\partial \bar{\rho} \tilde{R}_{ij}}{\partial t}}_{\text{ROC}} + \underbrace{\frac{\partial (\bar{\rho} \tilde{u}_k \tilde{R}_{ij})}{\partial x_k}}_{\text{convection}} = \underbrace{a_i \left( \frac{\partial \bar{p}}{\partial x_j} - \frac{\bar{\tau}_{jk}}{\partial x_k} \right) + a_j \left( \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \bar{\tau}_{ik}}{\partial x_k} \right)}_{\text{production}} - \bar{\rho} \tilde{R}_{ik} \frac{\partial \tilde{u}_j}{\partial x_k} - \bar{\rho} \tilde{R}_{jk} \frac{\partial \tilde{u}_i}{\partial x_k}$$

+ turbulent transport (unclosed) + pressure strain redistribution (unclosed) + dissipation (unclosed)

# Turbulent mass flux and density-specific-volume covariance

- $a_i = \overline{\rho' u_i'} / \bar{\rho}$ : velocity associated with turbulent mass flux
- To close  $\bar{\rho} a_i$ , BHR model by Besnard et al.<sup>26</sup> suggests to model transport of  $\bar{\rho} a_i$ :

$$\underbrace{\frac{\partial (\bar{\rho} a_i)}{\partial t}}_{\text{ROC}} + \underbrace{\frac{\partial (\bar{\rho} \tilde{u}_k a_i)}{\partial x_k}}_{\text{convection}} = \underbrace{b \left( \frac{\partial \bar{\rho}}{\partial x_i} - \frac{\partial \bar{\tau}_{ki}}{\partial x_k} \right) - \tilde{R}_{ik} \frac{\partial \bar{\rho}}{\partial x_k}}_{\text{production}} + \text{redistribution} \\ + \text{turbulent transport (unclosed)} + \text{destruction (unclosed)}$$

- $b = -\overline{\rho'(1/\rho)'}$ : density-specific-volume covariance
- BHR-3 model by Schwarzkopf et al.<sup>27</sup> recommends to model transport of  $\bar{\rho} b$ :

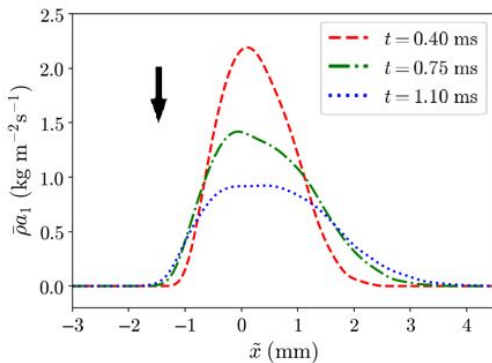
$$\underbrace{\frac{\partial \bar{\rho} b}{\partial t}}_{\text{ROC}} + \underbrace{\frac{\partial (\bar{\rho} \tilde{u}_k b)}{\partial x_k}}_{\text{convection}} = \underbrace{-2(b+1) a_k \frac{\partial \bar{\rho}}{\partial x_k}}_{\text{production}} + \text{redistribution} + \text{turbulent transport (unclosed)} \\ + \text{destruction (unclosed)}$$

<sup>26</sup>Didier Besnard et al. *Turbulence transport equations for variable-density turbulence and their relationship to two-field models*. Tech. rep. Los Alamos National Lab., NM (United States), 1992.

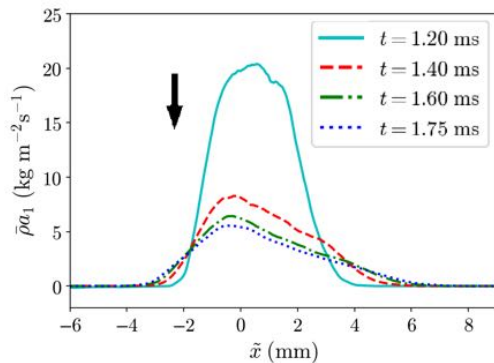
<sup>27</sup>John D Schwarzkopf et al. "Application of a second-moment closure model to mixing processes involving multicomponent miscible fluids". In: *Journal of Turbulence* 12 (2011), N49.

## Profiles of $\bar{\rho}a_1$ (in moving frame of interface)

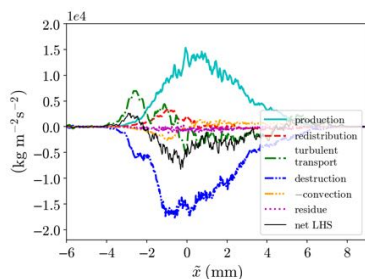
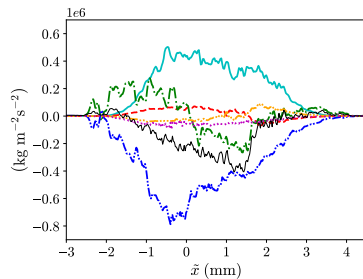
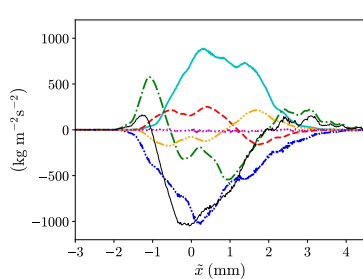
- Using highest Reynolds number 3D case in previous section
- $\tilde{x} = x - x_i$ , where  $x_i$  is location of interface
- After both first shock and re-shock,  $\bar{\rho}a_1$  spreads and the peak decreases over time



(a) After first shock, before re-shock



(b) After re-shock

Budget of turbulent mass flux,  $\bar{\rho}a_1$  (in moving frame of interface)(a)  $t = 1.10$  ms (before re-shock)(b)  $t = 1.20$  ms (after re-shock)(c)  $t = 1.75$  ms

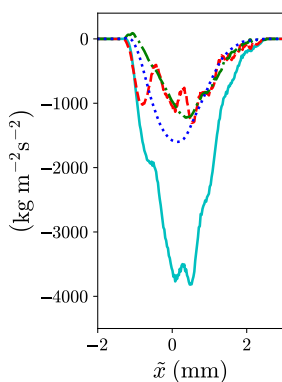
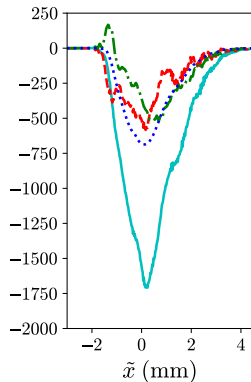
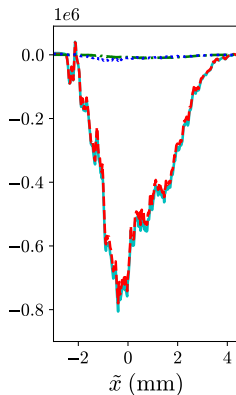
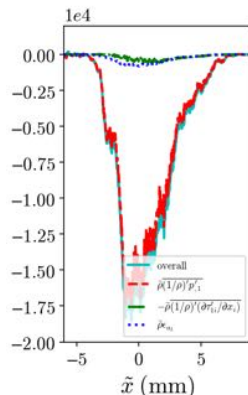
- The **production** and **destruction (unclosed)** terms are dominant terms in the budget
- The net LHS (rate of change + convection) is negative in the middle part of mixing layer, causing  $\bar{\rho}a_1$  to decrease in magnitude after first shock and re-shock
- **Turbulent transport (unclosed)** term spreads the profile
- **Redistribution** and **convection** terms are small over time

# Budget of turbulent mass flux, $\bar{\rho}a_1$

- Destruction** consists of three unclosed components:  $\bar{\rho}(1/\rho)'p'_{,1}$ ,  $-\bar{\rho}(1/\rho)'\tau'_{1i,i}$ ,

$$\bar{\rho}\epsilon_{a1} = -\bar{\rho}u'_i \frac{\partial u'_k}{\partial x_k}$$

- $\bar{\rho}(1/\rho)'p'_{,1}$  is the only important term after re-shock

(a)  $t = 0.40$  ms(b)  $t = 1.10$  ms  
(before re-shock)(c)  $t = 1.20$  ms (after  
re-shock)(d)  $t = 1.75$  ms

# Assessment of BHR-3<sup>29</sup> model: unclosed terms of transport equation of $\bar{\rho}a_1$

- Turbulent mass flux,  $\bar{\rho}a_1$ :

Unclosed Term	Exact Form	Modeled Form <sup>28</sup>
Turbulent transport	$-\bar{\rho} \frac{\partial (\overline{\rho' u' u'} / \bar{\rho})}{\partial x}$	$2C_a \bar{\rho} \frac{\partial \left[ (S \tilde{R}_{11} / \sqrt{k}) a_{1,1} \right]}{\partial x}$
Destruction	$\bar{\rho} \left( \frac{1}{\rho} \right)' \frac{\partial p'}{\partial x}$	$-C_{a1} \bar{\rho} \frac{\sqrt{k}}{S} a_1$

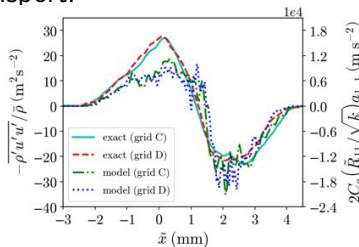
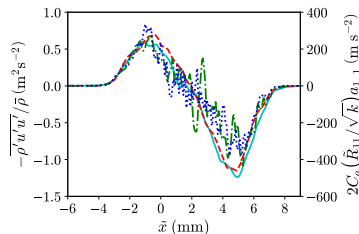
- $C_a$  and  $C_{a1}$  are model coefficients;  $S$  is a turbulent length scale
- Assuming  $S$  uniform inside mixing region (ignoring  $S$ ), cancelling common terms and operators for analyzing validity of model **after re-shock** (after mixing transition has occurred)

<sup>28</sup>  $k = \tilde{R}_{ii}/2$  is turbulent kinetic energy per unit mass

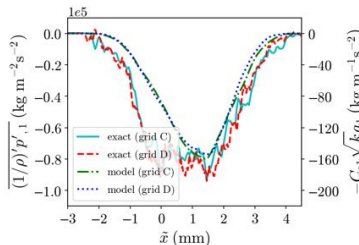
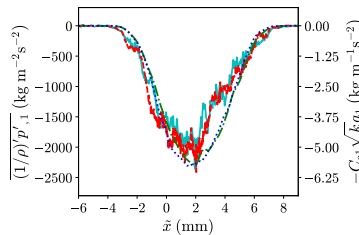
<sup>29</sup> Schwarzkopf et al., "Application of a second-moment closure model to mixing processes involving multicomponent miscible fluids".

# BHR-3 assessment: unclosed terms of $\bar{\rho}a_1$ transport equation (after re-shock)

- Turbulent transport:

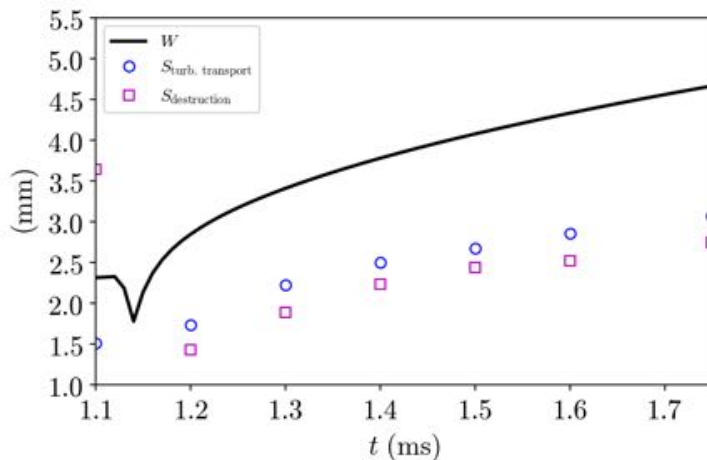
(a)  $t = 1.20$  ms(b)  $t = 1.75$  ms

- Destruction:

(a)  $t = 1.20$  ms(b)  $t = 1.75$  ms

## BHR-3 assessment: turbulent length scales $S$ (after re-shock)

- $W$ : integral mixing width
- **Least square fit** within mixing region to estimate  $S$ 's **required** for **turbulent transport** and **destruction** terms of  $\bar{\rho}a_1$
- Two length scale turbulence model BHR3.1 [Schwarzkopf et al., 2015] seems unnecessary for  $a_1$





# Summary

- $\bar{\rho}a_i$  plays an important role for modeling of  $\tilde{R}_{ij}$  in BHR-3 model
- $\bar{\rho}a_1$  transport equation was analyzed
- Destruction term in budget of  $\bar{\rho}a_1$  has different composition before and after re-shock (after mixing transition)
- BHR-3 model captures shapes of unclosed terms of  $\bar{\rho}a_1$  transport equation well
- $S$ 's required for modeling unclosed terms of  $\bar{\rho}a_1$  transport equation dependent on each other

Analysis of budgets and closures for  $\tilde{R}_{ij}$  and  $b$  discussed in thesis

# Conclusions

- High-resolution and localized dissipation schemes improved for shock problems that involve flow instabilities and turbulence
- AMR framework was developed and shown to be robust for problems that involve shocks and multi-species
- Asymmetric variable-density mixing effects examined
- Reynolds number has large effect on the flows before re-shock (before mixing transition)
- The BHR-3 model has good modeling assumptions for the  $\bar{\rho}a_1$  transport equation for post-transition flows

# Questions?

The PhD research was partially supported by Los Alamos National Laboratory, under grant number 431679.